TOPOLOGICAL ASPECTS OF PHASE TRANSITIONS

L. ROSS

Abstract. In the past decade and a half, an alternative analysis of phase transitions, based in the topological behavior of system configuration spaces, has been introduced. This method offers a new understanding of many phase transitions, particularly those in finite systems, using topology and manifold behavior. While the broadest hypotheses offered by researchers have proven overly optimistic, the methods proposed have proven useful in many cases and offer some intriguing insights into the origins of phase transitions.

1. Introduction

A fundamental difficulty in statistical mechanics has long been the problem of predicting phase transitions using traditional statistical methods, particularly in finite systems. Both sufficient and necessary conditions for phase transitions are in short supply, and those currently known tend to be either overly general or apply only to narrow ranges of systems. In 1997, Caiani et al, noting that certain properties of the metric spaces of Hamiltonian dynamics showed a correspondance with transition behavior, put forth the hypothesis that phase transitions could be linked to topological features of the underlying system phase space.[1] More specifically, the so-called topological hypothesis conjectured that phase transitions required the existence of a break in the diffeomorphism of the topology of the energy manifold (in configuration space) at the transition energy.

This suggestion, having reasonable theoretical underpinnings, led to a wave of research attempting to validate the hypothesis in the late 1990s and early 2000s. Topological properties are both broad and simple, reducing the amount of information involved in a problem to a fairly minimal level and thus offering an appealing way to identify phase transitions. Early research was quite promising, with several positive proofs for certain system types, and helped lead to further work. Later numerical experiments disproved the hypothesis as a universal statement, but prospects for many systems of interest (unlike most theoretical methods, the topological hypothesis works, in many ways, more cleanly with *finite* systems) remain good, and further work on the limits of the hypothesis continues. In fact, the limits of the topological hypothesis offer interesting insights into the varieties of phase transitions and may lead to a greater understanding of such phenomena. [3]

2. Initial Theorems and Results

Phase transitions, in general emerge from the nonanalytic behavior of certain functions of certain statistical ensembles. This makes them very difficult to study

Date: May 11, 2012.

in small systems, since the behavior of ensemble functions of finite systems is going to require the computation and summation of at least N and more frequently N^m terms. If one considers, however, the energy manifold of the system configuration space, the most clearly visible way for such nonanalytic behavior to emerge is via the topology of the manifold - e.g., if, in going from the subset of the manifold where the energy is bounded by E to the subset where the manifold is bounded by $E + \delta$, a change in the topology of the subset occurs, the discontinuous nature of this behavior seems likely to introduce a nonanalytic point.

The above observation was first made in 1997 by Caiani et al and was thoroughly intriguing.[1] The lack of any other obvious causes of nonanalytic behavior in the energy manifold (which fully represented the system) led to the hypothesis that all phase transitions were caused by such topology changes (or, for some, the more modest proposal that all phase transitions in *finite* systems were caused by such topology changes). This led to a burst of research into systems whose phase transition properties were already known, to see if their topological behavior agreed with more traditional methods.

In 2004, a theorem was produced giving a set of systems whose phase transitions must be triggered by topological changes [3] - e.g., a set of systems subject to a necessity theorem on phase transitions. Those systems whose potential interactions were confined to a finite neighborhood of each particle, and whose general potentials were smooth and confining (so energy submanifolds were at all finite energies compact) must, according to the Franzosi-Pettini Theorem, have phase transitions only at the points where topological discontinuies between energy submanifolds emerged.

3. Numerics and Further Results

A primary obstacle in assessing the accuracy and usefulness of the topological hypothesis is the difficulty of finding systems for which all relevant parameters can be computed. Even numerically, this is a difficult task; since the limits of the topological hypothesis are not yet well established, computations at this point need to compute phase transitions of ensembles by both traditional methods (e.g., via microcanonical entropy) and by topological methods, to determine if the two methods are in agreement. Having said that, some models have been numerically analyzed and offer information on the limits of the topological hypothesis.

A point of interest is the underpinnings of those phase transitions not affiliated with topological changes. If the nonanalyticity of the microcanonical entropy doesn't come from the topology of the phase space, where does it come from?
Several specific counterexamples have been analyzed, two of the first being the mean-field ϕ^4 and solid-on-solid models. Both of these systems fail one (and only one) of the necessary criteria in Franzosi-Pettini theorem, the first failing the requirement that the potential between particles be short-ranged, the second the criterion that the potential must be confining. In both of these cases, the functions showing nonanalytic behavior (and thus phase transitions) are themselves functions of smooth functions; however, both involve a maximization over one variable. This

maximization process can (and,in these systems does) introduce its own nonanalyticity. The analysis of this second form of phase transition is interesting, too, in that by previous work, such generators of phase transitions cannot exist in the class of systems considered by the Franzosi-Pettini Theorem.[3]

Several papers have also been published in the last few years offering an explanation for certain types of phase transitions in infinite systems[4, 5, 6]. In particular, the existence of certain kinds of saddle points in the potential energy (as viewed in the configuration space), specifically those whose numbers grow in an unbounded fashion as the thermodynamic limit is approached, seem to sometimes introduce phase transitions. A criterion establishing some cases for which a phase transition must necessarily result from such saddle points has also been introduced, providing one more puzzle piece in the understanding of the mathematical origins of phase transitions.[4]

4. Current State of the Field and Conclusions

The topological hypothesis remains in a state of limbo. While it has been validated for systems under certain constraints, the exact limits of its viability remain unknown. In-depth analysis of additional systems and further work on extending the number of systems which it covers may lead to further developments; the analysis of those systems which fail the hypothesis to better understand non-topological origins of phase transitions will also provide useful information.

An additional difficulty with the topological hypothesis is that, while easier to use for certain systems than traditional methods, it is still difficult and unwieldy to apply to numeric simulations of most systems. While certain systems not analytically solvable by traditional methods may yield more readily to topological methods, it is not a straightforward and general method of analyzing all systems. For all that topological methods require far less data to determine phase transitions (topological genus is really a very minimal piece of information), finding that smaller portion of data is not necessarily any simpler.

All that being said, regardless of its limitations, the topological hypothesis is a strong and valuable tool in understanding phase transitions. By offering an alternative means of attack and a method of study which yields more readily to finite systems than infinite, the topological hypothesis may allow greater understanding of systems no otherwise approachable. Additionally, the very notion of using the topology of the configuration space manifold to find the origin of thermodynamic function nonanalyticities offers a new way to look at the mathematics of phase transitions and may help inspire even more new ways to analyze and simulate statistical physics systems.

References

[1] Caiani, L et al, 1997, "Geometry of dynamics, Lyapunov exponents and phase transitions"', Phys. Rev. Lett. 79, 4361.
[2] Pettini, M., 2007, Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics, Interdisciplinary Applied Mathematics Vol. 33 (Springer, New York).
[3] Kastner, M., "Phase transitions and configuration space topology", Rev. Mod. Phys. 80, 167187 (2008).

[4] Kastner, M. and Schnetz, O., ”Phase Transitions Induced by Saddle Points of Vanishing Curvature”, Phys. Rev. Lett. 100, 160601 (2008) .

[5] Kastner, M. et al, ”‘Nonanalyticities of the entropy induced by saddle points of the potential energy landscape”, Journal of Statistical Mechanics Theory and Experiment 2008, P04025 (2008).

[6] Angelani, L. and Ruocco, G., ”Role of saddles in topologically driven phase transitions: The case of the d-dimensional spherical model ”, Phys. Rev. E 77, 052101 (2008).

[7] Franzosi, R., and M. Pettini, Theorem on the origin of phase transitions, Phys. Rev. Lett. 92, 060601 (2004).

[8] Fabrizio Baroni and Lapo Casetti, ”Topological conditions for discrete symmetry breaking and phase transitions”, J. Phys. A: Math. Gen. 39 529 (2006)

[9] Kastner, M., ”When topology triggers a phase transition”, Physica A 365, 128-131 (2006).